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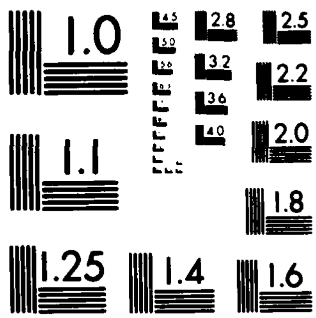

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NONLINEAR PROPERTIES OF MATERIALS
Final Report
(MDA-903-82-C-0053)

by

Bruce J. West
and
M.F. Shlesinger

30 Sept 82

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Supported by Defense Advanced Research Projects Agency

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1. INTRODUCTION

Investigation is made on

~~We proposed, under this contract, to investigate~~ such diverse phenomena as turbulence, extreme properties of stochastic systems, the statistics of nonlinear wave-wave interactions and the detection of clustered events. One of the theories developed to explain the transition from laminar to turbulent flow is through the use of intermittent turbulent bursts interacting with the laminar flow to generate more bursts and thus form a cascade to a fully developed turbulent state. Thus, the statistical distribution of such bursts is important in determining the rate of transition from laminar to turbulent fluid flow and can thereby strongly influence the drag properties of fluid flowing past a body. A second process in which intermittency is important is the anomolous transport of charge in amorphous materials. The current flow in these materials exhibits a clustering of events in time not unlike that observed in fluid turbulence. In both of these systems the physical observables, *e.g. the correlation function,* exhibit scaling behavior with exponents characteristic of the process. A final example is the stress relaxation of polymers, in which case the scaling behavior effects such material properties as brittleness, dielectric loss, etc. ~~Under this contract we have developed~~ a new random walk model is developed which greatly increases our understanding of such processes.

Many scaling relations for complex systems in the physical sciences involve non-integer exponents. We list several examples of these below, which although well known have provided us with the orientation necessary to investigate more unfamiliar physical situations. We interpret the non-integer exponents in the scaling relations as indications of singularities arising from probability distributions with long tails governing the physical observables. The existence of such distributions to describe turbulence, electron transport in amorphous materials and other areas has been proposed by a number of investigators. But

heretofore no systematic investigation of the physical implications of these distributions has been presented. The initial work in this area has been done under this contract in the sequence of fifteen papers described below.

If the first moment of the appropriate physical observable with respect to one of these long tailed distributions diverges, then no scale exists in which to gauge measurements and structure occurs on all scales. The concepts of self-similar fractals, non-differentiability , and also non-integer exponents all accompany the divergence of such low order moments. The analysis we have done centers around the construction of simple mechanical models exhibiting these properties. In particular we examine random walk examples where the above characteristics appear simply and naturally. These random processes have an inherent self-similar (fractal) scaling in space, time, frequency or other appropriate variable. They can be used to model complex systems of interest which exhibit features spanning many decades of scale. As mathematicians we categorize possible behaviors and as physicists we search for the basic interactions which lead to such behavior.

2. SURPRISES IN EXPERIMENTAL PHYSICS

When one begins the study of physics, one invariably discovers simple laws such as momentum (mv = constant) conservation and energy conservation ($\frac{1}{2}mv^2 = constant$). One also encounters many well-defined concepts, such as the mobility μ, ($\vec{v} = \vec{\mu} \cdot \vec{E}$), say for a conductance electron in a metal. Simple relations are ubiquitous, e.g., the mean square displacement of a random walker after N steps is proportional to N; the vibrational density of states $\rho(\omega)$ of a D dimensional crystal at low frequencies scales as ω^{D-1}, etc. Everywhere exponents seem to be integers and quantities are well-defined.

When one deals with actual systems which are sufficiently complex, it is often the case that the best description is in terms of probability distributions. A Poisson distribution is characterized by its first moment, and a Gaussian distribution by its first two moments. When distribution have long enough tails, the first few moments will not characterize the distribution. Distributions with infinite moments will lead to physics described by non-integer exponents, and to surprises which run counter to our intuition. We list some examples which we have investigated where non-integer exponents abound.

A. High Velocity Impacts[1,2]

An important materials science problem is the effect of high velocity micro meteorites (mass m, velocity v) on spacecraft. As a result of a collision many interesting phenomena occur, deformation of the meteor, (projectile) crater formation on the surface of the spacecraft (target), shock wave generation, melting, and crack propagation. One would suspect that the crater formed by the collision would be proportional to the kinetic energy of the meteor ($\frac{1}{2}mv^2$) leading to the radius of the crater R scaling as $R^3 \sim v^2$. Momentum conservation is not considered because target material is thrown backwards during the

crater formation thus enhancing the forward momentum. The surprise is that the crater depth scales as a power of the velocity, i.e.

$$R \sim v^{\alpha} \ , \ \alpha = 0.58 \tag{1}$$

but $\alpha \neq 2/3$. This implies a new conservation law given by

$$mv^{1.74} = constant \ . \tag{2}$$

We have been able to explain this scaling behavior by using a random walk model for the movement of dislocations in the target material.

B. Charge Transport in Amorphous Films[3-5]

In the xerographic process a flash of light creates a layer of electron-hole pairs in an amorphous film. The charges separate under the influence of an external electronic field E. If the film is of depth L, and there exists a mean transit time T for charges to cross the film, then one expects that $L/T = \mu E$. Instead one finds (for a-As_2 Se_3) that

$$T^{-1} \sim (E/L)^{2.2} = (E/L)^{1/.45} \tag{3}$$

for a wide variety of E and L values. The current I(t) generated by the charge movement is found to have two regimes. In the early phase

$$I(t) \sim t^{-1+.45} \tag{4a}$$

and in the late phase (caused by absorption at the far surface)

$$I(t) \sim t^{-1-.45} \tag{4b}$$

A continuous time random walk model is the only complete description of this phenomenon.[18]

C. Polymers[6]

1. The world of polymers is full of fractional exponents. The mean square displacement $< R^2 (N) >$ of a self-avoiding random walk (SAW) after N steps can be used to model the end-to-end distance of a polymer, in a good solvent. In three dimensions (3D)

$$< R^2(N) > \sim N^\gamma \quad (5)$$

with $\gamma \sim 1.2$. Mandelbrot[7] has suggested that $\gamma = 2/\mu$ where μ is the "fractal" dimension of the SAW and is approximately[8] $\ln 6/\ln 3 \sim 1.6$. Shlesinger[8] has used some recent results of Seshadri and West[21] to explain this phenomenon using the newly developed concept of fractal random walks developed under this contract[8,12,15,18]

2. The vibrational density of states $\rho(\omega)$ of certain proteins is found at low frequencies to be[9]

$$\rho(\omega) \sim \omega^{.65 \pm .04} \quad (6)$$

This is consistent with the protein having a 3D SAW shape and $\rho(\omega) \sim \omega^{\mu-1}$, and in contrast to the Debye law $\rho(\omega) \sim \omega^{D-1} = \omega^2$ in 3D.

3. The repetition time τ_R for polymer melts is defined as the cross-over time from rubber-like to liquid-like behavior. It is found to scale with polymer mass M as

$$\tau_R \sim M^{3.3} \quad (7)$$

A simple diffusion model[6] for the motion of constrained polymer chains would yield $\tau_R \sim M^3$.

4. The dielectric response of polymers (as well as many other materials) is governed by non-integer exponents. The frequency dependent dielectric constant $\varepsilon(\omega)$ is given by

$$\frac{\varepsilon(\omega) - \varepsilon_\infty}{\varepsilon_\infty - \varepsilon_0} = -\int_{-\infty}^{\infty} e^{-i\omega t} \frac{d\varphi(t)}{dt} dt \quad (8)$$

Williams and Watt[10] find that a good form for the response function is

$$\varphi(t) = Ae^{-Bt^\alpha},\ 0<\alpha\leq 1 \quad (9)$$

The relation between this response function and long tail distributions has been discussed in some detail by Montroll and Shlesinger.[16]

5. Amorphous solids are not in thermodynamic equilibrium at temperatures below their glass transition temperature. These non-equilibrium states are metastable and slowly relax towards equilibrium and in so doing affect many properties of the material, e.g. the material becomes stiffer and more brittle, its damping decreases and so do the creep- and stress-relaxation rates, the dielectric constant, the dielectric loss etc. The lifetime of such metastable states when the transition is induced by correlated fluctuations has been studied by West and Lindenberg.[19,20] The probability density in this case is shown to satisfy a Fokker-Planck equation having a diffusion coefficient which is both time dependent and dependent on the state of the system.

3. FROM NON-INTEGER EXPONENTS TO SELF-SIMILARITY

Integer exponents can usually be traced back to the analytic behavior of an appropriate function which can be expanded in a Taylor series. Non-integer exponents imply the presence of singularities and the breakdown of a Taylor series due to the divergence of a coefficient. ***Our main theme is that singularities and thus non-integer exponents arise in complex systems because they exhibit randomness on many scales.*** As an example, consider the probability $\psi(t)\,dt$ for an event (electron hopping, dislocation movement, crack propagation, etc.) to occur in the time interval (t, t+dt). Its Laplace transform is defined by

$$\psi^*(s) \equiv \int_0^\infty e^{-st}\,\psi(t)dt \quad . \tag{10}$$

If all the moments $<t^n>$ of $\psi(t)$ exist, then

$$\psi^*(s) = 1 + \sum_{n=1}^{\infty} \frac{(-s)^n}{n!} <t^n> \tag{11}$$

and times will be measured in units of <t>. If however, <t> is infinite, i.e.,

$$<t> = \sum_0^\infty t\,\psi(t)dt = -\frac{\partial}{\partial s}\psi^*(s=0) = \infty$$

then t/<t> is not an appropriate dimensionless time, and $\psi^*(s)$ cannot be represented in a Taylor series about s = 0. This will occur if at long times $\psi(t) \sim t^{-1-\alpha}$, $0 < \alpha < 1$. A proper small s expansion[3-5,11] of $\psi^*(s)$ will include an s^α term. Effectively t is replaced by t^α in all dimensional analysis. This is the underlying cause for the non-integer exponents in (3) and (4). Such $\psi(t)$ arise from a distribution of deep traps in the material which can capture charges in amorphous materials,[3-5] dislocations in elastic materials[2,23] and/or excitations in polymers.[26,27] There is no average time in these problems when <t> = ∞, so that the duration between events occurs on all time scales. A self-similar set of burst of events has this property.

Systems with inherent scaling are most naturally described by scaling equations, and not by differential equations. In fact, the appropriate functions may be nowhere differentiable. Scaling brings us into the province of the renormalization group (RNG).[11] Let us consider how the free energy F of a system scales near a critical point.

Let K describe interactions within a small system, and K'(K) interactions between these small systems. When a non-trivial fixed point of the RNG transformation K'(K) = K exists, one may switch to a scaling variable, u, to find

$$F(u) = l^{-D} F(\lambda u) + G(u) \tag{12}$$

where in D dimensions, u describes the small system of unit size, λ u the larger system of size l^D, λ is a relevant eigenvalue of the RNG transformation, and G is an analytic function. Let us iterate (12) n times and then let n $\to \infty$, to obtain

$$F(u) = \lim_{n \to \infty} \left[l^{-nD} F(\lambda^n u) + \sum_{j=0}^{n-1} l^{-jD} G(\lambda^j u) \right] . \tag{13}$$

It is usually assumed that the fist term on the rhs vanishes as n $\to \infty$, and thus all singularities in F(u) must shift to the term involving the summation over G. A solution to the singular part of (13) is

$$F(u) = A(u) | u |^{D \ln l / \ln \lambda} \tag{14a}$$

where A(u) is oscillatory in ln u with period ln λ, i.e.

$$A(u) = A(\lambda u) = \sum_n A_n e^{2\pi i n \ln u / \ln \lambda} \tag{14b}$$

In our work we introduced fractal random walks[11-15] processes which produce non-integer exponents naturally in the form of fractal dimensions, and integral transforms of probability distributions exhibit precisely the scaling of (12) - (14).

We treat separately the most famous scale-invariant problem the "1/f noise" problem.[16,17,18] For many diver e systems the power spectrum S(f)

(the Fourier transform of a second order correlation function C (t)) has a low frequency component scaling as the inverse of the frequency, i.e.

$$S(f) = \mathrm{Re}\int_0^\infty e^{2\pi i f t}\, C(t)dt \sim 1/f \ \ as\ f \to 0$$

In this regime the integrated power spectrum is independent of scale, i.e.

$$\int_{f_{min}}^{f_{max}} \frac{df}{f} = \int_{f_{min}}^{f_{max}} \frac{d(f/f_0)}{f/f_0}$$

For a completely random system $C(\tau) = e^{-t/\tau}$ where τ is a relaxation time. In a complex system a distribution of relaxation times $\rho(\tau)$ can exist. Then

$$S(f) = \int_0^\infty e^{2\pi i f t}\, e^{-t/\tau} \rho(\tau) d\tau \ .$$

If $\rho(\tau) \sim \tau^{-1}$ then a regime of 1/f noise will result. We show that such a $\rho(\tau)$ arises when the probability of fluctuation depends on the product of several random variables.[16] In this case $\rho(\tau)$ will be a log-normal distribution in contrast to the normal distribution which arises for the distribution of a sum of random variables. Our $\rho(\tau)$ involves a geometric mean while the normal distribution involves a arithmetic mean.

The log normal distribution also describes (at longer times) the lifetime of many materials. We are at present investigating deviations to this law at early times.

The random walk models developed to understand the phenomenon of clustering in either space and/or time have relied on long range transition probabilities for stepping between sites on a lattice. In the continuum limit the probability density has been shown to satisfy an integral-differential equation rather than a Fokker-Planck equation.[12,14,15] The solutio.ı to this equation is a Lévy distribution having the characteristic function $\varphi(\mathbf{k}) = e^{-\gamma|\mathbf{k}|^{\mu}}$ i.e. the Fourier transform of the probability density. The Lévy distribution describes intermittent or clustered processes having mean first passage times and maxima

moments which scale with the characteristic exponent μ.[21,22] The Lévy parameter μ has been identified with the fractal dimensionality for the process[21] and can be expressed in terms of the random walk parameters.[12,15] This identification has been used in both the high-velocity impact problem[2,23] and the end-to-end distance of a polymer chain[8].

The dynamic equations describing the evolution of such systems are necessarily nonlinear and stochastic, as for example the description of the generation and evolution of dislocations in elastic materials.[24] The analysis of such nonlinear stochastic equations is notoriously difficult so we have also developed under this contract a linearization method which is *instantaneously optimal* at all stages of evolution of the process. Detailed comparison of the results of this technique with Monte Carlo calculations on certain model systems are presented by West, et. al.[25] and the comparison is quite favorable.

Energy transport in molecular aggregates, e.g. polymeric materials, has long been a useful diagnostic for the determination of their structural and dynamical properties. One of the serious limitations of the previous theories has been the lack of understanding of the temperature dependence of the measured transport properties of the aggregates. The limitation arises precisely because these have been infinite temperature theories. West and Lindenberg[26,27] have developed a novel approach for the incorporation of finite temperature effects into a phenomenologically based model. By including the appropriate dissipative effects in the equations for exciton dynamics in molecular aggregates, the new theory is correct at finite (arbitrarily low) temperatures and indications are that it will be able to explain a number of "anomolous" temperature dependencies of spectral and transport properties.

REFERENCES

Note: All references preceeded by an asterisk have been completed under the present contract.

1. J.K. Dienes and J.M. Walsh in *High Velocity Impact Phenomena*,, R.Kinslow, ed. Academic Press, NY, (1979).

*2. B.J. West and M.F. Shlesinger, "Random walk of dislocations following a high-velocity impact," J. Stat. Phys. **30**, 547 (1983).

3. E.W. Montroll and H. Scher, J. Stat. Phys. **9**, 101 (1973).

4. M.F. Shlesinger, J. Stat. Phys. **10**, 421 (1974).

5. H. Scher and E.W. Montroll, Phys. Rev. **B12**, 2455 (1975).

6. P.G. de Gennes, *Scaling Concept in Polymer Physics* Cornell University, Ithaca, (1975).

7. B.B. Mandelbrot, *The Fractal Geometry of Nature*, W.H. Freeman, San Francisco, (1982).

*8. M.F. Shlesinger, "Weierstrassian Lévy Flights and self-avoiding random walks," J. Chem. Phys. **78** 416 (1983).

9. H.T. Stapeleton, T.P. Allen, C.P. Flynn, D.G. Stenson and S.R. Kurtz, Phys. Rev. Lett. **45** 1456 (1980).

10. G. Williams and D.C. Watt, Trans. Faraday Soc. **66**, 80 (1970).

11. M.F. Shlesinger and B.D. Hughes; "Analogs of Renormalization Group Transformations in Random Processes," Physica **109A**, 597 (1981).

*12. B.D. Hughes, E.W. Montroll and M.F. Shlesinger; "Fractal Random Walks," J. Stat. Phys. **28**, 111 (1982).

*13. B.D. Hughes and M.F. Shlesinger, "Lattice Dynamics, random walks, and nonintegral effective dimensionality," J. Math. Phys. **23**, 1688 (1982).

*14. M.F. Shlesinger, J. Klafter and Y.M. Wong, "Random walks with Infinite Spatial and Temporal Moments," J. Stat. Phys. **27**, 499 (1982).

*15. B.D. Hughes, E.W. Montroll and M.F. Shlesinger, "Fractal and Lacunary Stochastic Processes," J. Stat. Phys. **30**, 273 (1983).

*16. E.W. Montroll and M.F. Shlesinger, "Maximum entropy formalism, fractals, scaling phenomena and 1/f noise: A Tale of Tails," to be published, (LJI-R-83-225).

*17. "On 1/f noise and other distributions with long tails," Proc. Nat. Acad. Sci. USA **79**, 3380 (1982).

*18. E.W. Montroll and M.F. Shlesinger, "A wonderful world of random walks," to be published (LJI-R-83-221).

*19. K. Lindenberg and B.J. West, "Finite Correlation Time Effects in nonequilibrium phase transitions I. Dynamic Equations and steady state properties," to appear in Physica (1983) (LJI-R-83-220).

*20. B.J. West and K. Lindenberg, "Fokker-Planck description of Multi-degree-of-freedom systems with correlated fluctuation," to appear in Phys. Lett. (1983) (LJI-R-82-222).

21. V. Seshadri and B.J. West,"Fractal dimensionality of Lévy Processes," Proc. Natl. Acad. Sci. USA **79**, 4501 (1982).

*22. B.J. West and V. Seshadri, "Linear Systems with Lévy Fluctuations," Physica **113A**, 203 (1982).

*23. B.J. West and M. Shlesinger, "Random Walk Models of Impact Phenomena," to be published (LJI-R-82-183R).

24. K. Kawata and J. Shioiri, editors, *High Velocity Deformation of Solids*, IUTAM Sym., Springer-Verlag, Berlin (1978).

*25. B.J. West, G. Rovner and K. Lindenberg, "Approximate Gaussian representation of evolution equations I. Single degree of freedom nonlinear equations," J. Stat. Phys. **30**, 633 (1983).

*26. B.J. West and K. Lindenberg, "Stochastic Model of Exciton Lineshapes at Finite Temperatures" to appear in *Random Walk Models in Physical and Biological Systems*, editors M. Shlesinger and B.J. West, AIP Conf. Proceed. (1983) (LJI-R-83-234).

*27. K. Lindenberg and B.J. West "Exciton Lineshapes at Finite Temperatures," to appear in Phys. Rev. Lett. (1983) (LJI-R-83-239).